On the Accuracy of Parameters Derived from Permeation and Diffusion Experiments - 10134

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ABSTRACT

Safety assessment of facilities associated with geological disposal of hazardous waste, including radioactive nuclear waste, is generally performed through mass transport simulations combined with uncertainty and sensitivity analyses. To reduce the uncertainty of a simulation, mathematical models describing the mechanisms of mass transport in a geological formation and boundary conditions describing the geological and hydro-geological conditions for a specific site should be pertinent. In addition, the values of parameters input for the simulation should be representative of those under *in situ* conditions. Although both laboratory permeation and diffusion experiments have long been used in practice, and are considered to be well-established approaches for characterizing the hydraulic and diffusive properties of geological materials, they do not necessarily provide accurate values of parameters to be determined without careful examination of calculation and/or test conditions. Taking the transient pulse permeability test and the through-diffusion test as examples, this paper discusses some major factors that may cause errors in parameter determination. Our discussions indicated that: 1) although it is not a technical problem, negligence or some simple mistakes could be easily made in a calculation due to the use of different mathematical functions and/or unit systems; 2) compressibility of a permeation system is significantly larger than the nominal values for water due to the mechanical compliance of the equipment. The use of nominal values for the compressibility of water to calculate the value of permeability by using a simplified approach may significantly underestimate the permeability; 3) neglecting the effects of specific storage may overestimate or underestimate the permeability from a pulse test, depending on the relationships between the storage capacities of the specimen and reservoirs, and simplified equations being used; 4) the use of simplified solution together with the conventional time-lag method for the through-diffusion test may underestimate both the effective diffusion coefficient and rock capacity factor derived. The higher the concentration increase in the measurement cell, the larger will be the error in estimating the two parameters. To obtain reliable values for related parameters, caution should be exercised when interpreting data derived from the transient pulse permeability test and the through-diffusion test.

INTRODUCTION

Safety assessment of facilities associated with geological disposal of hazardous waste, including radioactive nuclear waste, is generally performed through mass transport simulations combined with uncertainty and sensitivity analyses. To reduce the uncertainty of a simulation and/or to increase the reliability of an analysis, mathematical models describing the mechanisms of mass transport in a geological formation and boundary conditions describing the geological and hydro-geological conditions for a specific site should be pertinent. In addition, the values of parameters input for the simulation should be representative to those under *in-situ* conditions [1].

Transport of contaminants, such as radionuclides, through an engineered and natural barrier system is primarily controlled by advection, dispersion, sorption, chemical and/or biochemical reactions, and chain decay [1-4]. Parameters related to the first five mechanisms are generally determined through permeation,

diffusion and batch experiments, and parameters related to the last mechanism are known in general and can be determined from nuclear physics [1].

Although permeation, diffusion as well as batch experiments have long been used in practice, and are generally considered to be well-established approaches for characterizing the hydraulic, diffusive and adsorptive properties of geological materials, they do not necessarily provide accurate values of parameters to be determined without careful examination of calculation, test conditions as well as other factors like resolution of analytical equipment

Taking the transient pulse permeability test, a method that has been widely used for testing low-permeability materials like engineered and natural barrier materials in geotechnical and/or geo-environmental laboratories, and the through-diffusion test, one of the methods that has been widely used in the field of waste management, as examples, this paper discusses some major factors that may cause errors in parameter determination. The purposes of this paper is to provide some practical considerations for effective implementations of laboratory permeation and diffusion tests, proper interpretation of test results, examination and/or proper citation of the data reported in existing articles for a scientific simulation.

TRANSPORT PROPERTIES OF GEO-MATERIALS

In general, the transport properties of a geo-material primarily include the hydraulic and diffusive properties. The hydraulic properties are represented by two parameters, called the permeability (or hydraulic conductivity) and specific storage. The diffusive properties are also represented by two parameters, called the effective diffusion coefficient and rock capacity factor. The magnitudes of these parameters are basically controlled by the porosity, connectivity, compressibility of individual mineral grains, and compressibility of bulk matrix of a geo-material. Many factors, such as rock type, geological process and other physicochemical properties, can affect the magnitudes of transport capacities [5].

Rock Type

The differences in rock type, or origins, may cause significant differences in transport properties of geo-materials. For instance permeability can range from more than 10^{-1} cm/s, for gravel formations to less than 10^{-9} cm/s for clay and igneous rocks. The difference in permeability of different rock types may therefore vary over ten orders of magnitude. It is not unusual that the permeability of the same rock type varies over three orders of magnitude due to the differences in microstructures within the rocks [6, 7]. In addition, heterogeneity and anisotropy are often observed in practice within a same rock formation. Although reports about systematic studies on effective diffusion coefficients of different rock types are generally not available because diffusion tests are more complicated and time-consuming than permeability tests, similar differences in the effective diffusion coefficient for different rock types may occur. The reason is that both the permeability and the effective diffusion coefficient are controlled by the same key physical parameters of a rock, i.e., the porosity and effective connectivity. Besides the connected pores, dead pores and/or fissures in a geo-material can storage fluid and chemical species, and thus affect the magnitude of specific storage and rock capacity factor.

Geological Process and Interrelationships between Different Properties

Geological process may induce significant changes in transport properties of a rock formation. Physical mechanical, thermo-dynamical, and chemical/biochemical evolutions within a geo-formation may cause changes in hydraulic and diffusive (i.e., the mass transport) properties. The four properties, i.e., the mechanical, chemical, thermal and mass transport properties, are interrelated. Changes in one property may introduce direct and indirect effects on other three properties. The interrelationships between the four properties together with major influential phenomena are depicted in Fig. 1 [5].

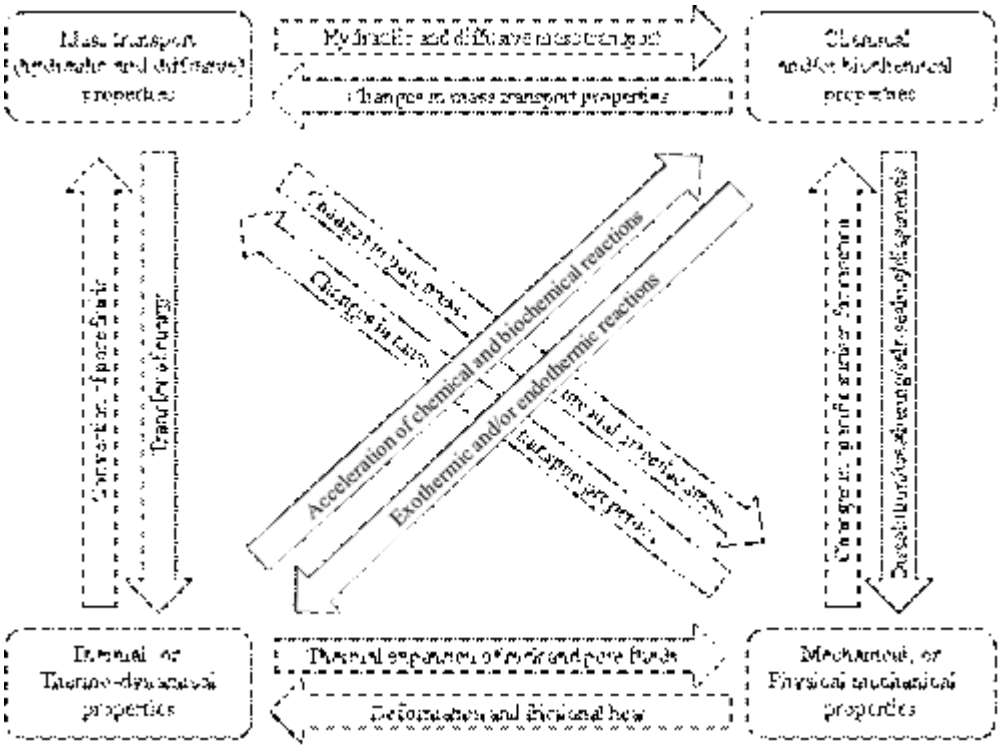


Fig. 1 Interrelationship between the mass transport, chemical, thermal and mechanical properties

Chemical evolutions within a geo-formation may induce changes in porosity and connectivity, and thus the mass transport properties. Adversely, hydraulic flow of groundwater and/or diffusive migration of chemical species within a geo-formation may induce chemical reactions. For example, mineral deposition and/or crystallization may decrease the porosity and connectivity, and thus the mass transport properties. Inversely, dissolution of minerals may increase the porosity and connectivity, and thus the mass transport properties.

Changes in mechanical properties may induce deformation in a geo-formation, and alter its mass transport properties. Inversely, the existence of groundwater may induce changes in pore pressure and effective stress, and affect the mechanical properties. For example, compression and/or consolidation of a geo-formation may induce a decrease in porosity or transport properties, and generation of abnormal pore pressures. Inversely, dilatancy and fractures induced during deformation of a geo-formation may cause increase in mass transport properties.

Thermal convection within a geo-formation may induce flow of pore fluids and thus mass transport. Inversely, the flow of pore fluids may cause redistribution of thermal energy and affect the thermal properties.

The interrelationships between different properties are complicated, depending on rock types, structural geological and hydro-geological boundary conditions. The time period required for a long-term performance assessment of a facility associated with geological disposal of high level radioactive waste (HLW) is generally in the order of several tens of thousands of years. Changes in transport properties over such a long time of geological process should be considered, but systematic knowledge that can be used for predicting the long term performance of a geological disposal facility with firm confidence is lacking.

Human Interruption

Human interruption will induce changes in individual properties of a geo-formation. Boring of holes for geological and hydro-geological investigations down to the depth at which a geological disposal facility is planned, and excavation of rock mass for the construction of an underground facility can be considered as typical examples of human interruption. Boring and excavation will cause stress release, stress redistribution, and excavation disturbed zone (EDZ) around boring holes, shafts and tunnels. The refill of boring holes can be difficult. The compatibility of refilling material with surrounding rock mass is one of key factors that control the long term performance of a facility.

Pumping of water during excavation and construction of an underground facility, and ventilation in shafts and tunnels may cause changes in groundwater level, oxidation and reduction conditions of pore fluids, and alter the mass transport properties of the geo-formation.

The emplacement of HLW into a geological disposal facility can also be considered as a type of human interruption on the geo-formation in which a facility is constructed. The heat generated from emplaced HLW may change thermal properties of surrounding rock mass and thus affect the mass transport properties both directly and indirectly.

Although coupled thermal, hydraulic, mechanical, and chemical (T-H-M-C) models have been proposed and developed based on some ideal assumptions, a systematic study is still of fundamental necessity for a full understanding of the mechanism and interrelationships between different properties. In addition, experimental data necessary for quantitative evaluations of the effects of individual factors on mass transport properties of geo-materials are limited.

Experimental Technologies

For testing a given rock sample under a given test condition, the accuracy of the parameters to be derived from a test would be affected by the test method itself. Major factors that may affect the accuracy of a test include the accuracy of equipments used for controlling test conditions, the sensitivity and accuracy of sensors and/or equipments used for detecting or analyzing related physical and chemical parameters, simplification of analytical models and test conditions, and possibly the human errors.

Taking the transient pulse permeability test and the through-diffusion test as examples, the following chapter discusses the accuracy of parameters derived from permeation and diffusion experiments.

PERMEATION AND DIFFUSION EXPERIMENTS

Similarity between Permeation and Diffusion

Permeation through and diffusion in a geo-material can be described with Darcy's law and Fick's second law, respectively. Combining the principle of mass conservation and the two laws, one dimensional transient flow and one dimensional diffusion through a saturated porous medium can be described by the following equations (1) and (2), respectively.

$$\frac{\partial^2 h}{\partial x^2} - \frac{S_s}{K} \cdot \frac{\partial h}{\partial t} = 0 \tag{1}$$

$$\frac{\partial c}{\partial t} = \frac{D_e}{\alpha} \frac{\partial^2 c}{\partial x^2} \quad \text{or} \quad \frac{\partial^2 c}{\partial x^2} - \frac{\alpha}{D_e} \cdot \frac{\partial c}{\partial t} = 0 \tag{2}$$

Where h, specifically $h(x,t)$, is the hydraulic head in the specimen, S_s and K are the specific storage and the permeability of the specimen, c or $c(x,t)$ is the concentration in the specimen, α and De are the rock capacity factor and the effective diffusion coefficient of specimen, x is the distance and t is the time.

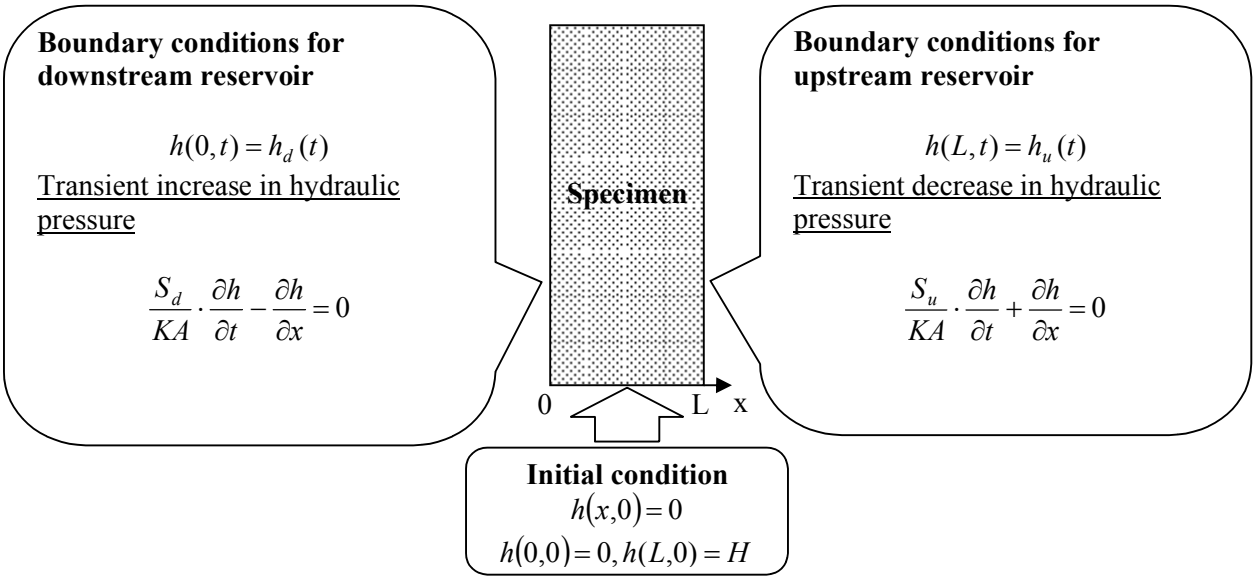
It is obvious that the governing equations or mathematical expressions for describing the permeation and diffusion within a geo-medium are quite similar to each other.

The transient pulse method was originally introdued by Brace et al. [8] for measuring low permeabilities in hydraulically tight rocks. The basic concept of the transient pulse technique involves connceting the specimen ends to two fluid reserviors, instantaneously increasing the fluid pressure in one reservior (upstream reservior), and measuring the corresponding pressure decay across the entire length of the specimen. The permeability, or hydraulic conductivity, and specific storage are then calculated directly from the record of decay in pressure pulse [8, 9, 10].

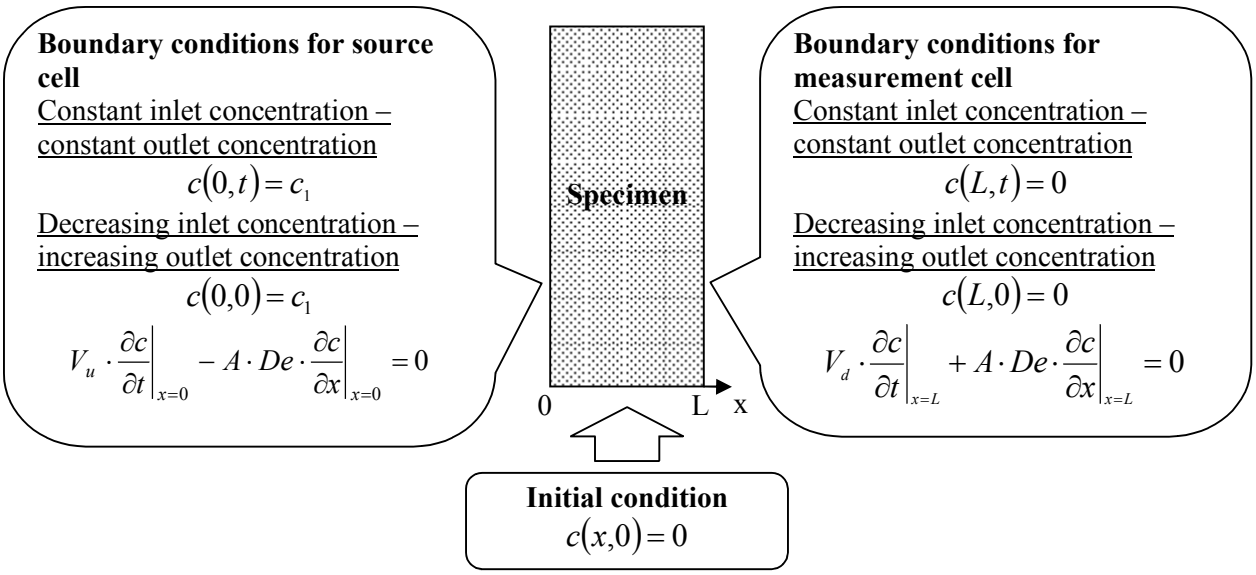
Quite similar to the transient pulse technique, the basic concept of the through-diffusion test involves sandwiching the test specimen between two reservoirs or cells. One of the reservoirs serves as the source reservoir spiked with the trace solute of interest and the other serves as the measurement reservoir. Changes of solution concentrations in the measurement and/or source reservoirs are monitored, and the effective diffusion coefficient and the rock capacity factor are then calculated from the measured data [2, 11].

Schematic diagrams illustrating the initial and boundary conditions for the transient pulse permeability test and the through-diffusion test are depicted in Fig. 2 a) and b), respectively. Where H is the instantaneous step increase in hydraulic head, S_d and S_u are the compressive storages of the downstream and upstream reserviors for the permeability test. And c_1 is the initial concentration in the source cell, Vu and Vd are the volumes of source and measurement cells or reservoirs for the diffusion test. A and L are the cross-sectional area and the length of specimen, respectively.

Transient decrease in hydraulic pressure within the upstream reservoir during a transient pulse permeability test is due to the outflow of water from the upstream reservoir into the specimen end connected to it. And the transient increase in hydraulic pressure within the downstream reservoir is due to the inflow of water from opposite end of the specimen into the downstream reservior (Fig. 2 a). Similarily, the time-dependent decrease of the tracer concentration within the source cell during a diffusion test is due to the migration of tracer from the source cell into the specimen end connected to it. The time-dependent increase of the tracer concentration within the measurement cell is due to the migration of tracer species from the opposite end of specimen into it (Fig. 2 b). It is quite easy to find again the similarity between the transient pulse permeability test and the through-diffusion test by comparing the schematic diagrams, intital and boundary conditions, and the expressions describing the initial and boundary conditions for individual tests.



a) Transient-pulse permeability test



b) Through-diffusion test

Fig. 2 Schematic diagrams and initial and boundary conditions for transient pulse permeability test and through-diffusion test

Examination of Transient Pulse Permeability Test

Exact or rigorous solution to the transient pulse permeability test can be obtained by solving the equation (1) together with the initial and boundary conditions illustrated in Fig. 2 a). Exact solution in dimensionless form has been derived by Hsieh et al. [9]. To facilitate understanding, the author prefers an explicit expression as follows [10]:

$$\frac{h(x,t)}{H} = \frac{1}{1+\beta+\gamma} + 2\sum_{m=0}^{\infty} \frac{\exp\left(-\frac{K\cdot\phi_m^2}{S_s\cdot L^2}\cdot t\right)\cdot\left[\cos\left(\phi_m\cdot\frac{x}{L}\right)-\frac{\gamma\cdot\phi_m}{\beta}\cdot\sin\left(\phi_m\cdot\frac{x}{L}\right)\right]}{\left[1+\beta+\gamma-\frac{\gamma\cdot\phi_m^2}{\beta}\right]\cos(\phi_m)+\left[1+\gamma+\frac{2\gamma}{\beta}\right]\phi_m\cdot\sin(\phi_m)} \tag{3}$$

In which $\beta = (S_s \cdot A \cdot L)/S_u$, $\gamma = S_d / S_u$ and ϕ_m are the roots of the following equation:

$$\tan(\phi) = \frac{(\gamma+1)\cdot\phi}{\gamma\cdot\phi^2/\beta - \beta} \tag{4}$$

Simplified solution to the transient pulse permeability test, neglecting the effects of specific storage of test specimen, was derived by Brace et al. [8], as expressed in the following equations:

$$h_u - h_f = H \cdot \frac{V_d}{V_u + V_d} \cdot e^{-\theta t} \tag{5}$$

where

$$\theta = (K\cdot A/\rho\cdot\lambda\cdot L)(1/V_u + 1/V_d) \quad \text{or} \quad K = (\theta\cdot\rho\cdot\lambda\cdot L\cdot V_u\cdot V_d)/[A\cdot(V_u+V_d)] \tag{6}$$

H_f is the final hydraulic head, V_u and V_d are the volumes of the upstream and downstream reservoirs, respectively, ρ is fluid density, and λ is the fluid compressibility. Note that some of the symbols used here to represent the physical parameters are different from those used by Brace et al. [8]. The permeability, or hydraulic conductivity with a unit of *L/T*, rather than the intrinsic permeability with a unit L^2, is used in this paper.

In most laboratories, same-sized pressure reservoirs are generally used, and the pressure decay is monitored across the entire length of test specimen using a differential pressure transducer with relatively high sensitivity and precision. In this case, h_f can be assumed to be the average of h_u and h_d. Equation (5) can then be reduced to the following equation (7) :

$$\frac{h_u - h_d}{H} = e^{-\theta t} \tag{7}$$

The solution for the pressure decay within the upstream reservoir, h_u-h_f, is exponential. To determine the value of θ from an experimental record, $(h_u - h_f) \cdot (V_u + V_d) / (H \cdot V_d)$ should be plotted as the natural log versus time. If the observed pressure decay is plotted against time, simply due to a mistake in calculation, the slope of $-\theta$ becomes 2.3 times smaller than plotted on the semi-natural log axis versus time. Such a simple mistake was made in the article written by Brace et al. [8] who originally introduced the transient pulse technique, and this article has been referred by many researchers who are not necessarily aware of this mistake. If other calculations were correct, the values of permeability of Westerly granite reported by Brace et al. [8] should be multiplied by a factor of 2.3.

The value of permeability calculated from equation (6) is propotional to the value of fluid compressity, or more exactly, the compressibility of permeation system that is controlled by both the compressibity of water and mechanical compliance of the equipment, or tubing system. The compressibity of permeation system depends on the stiffness of tubing system, concentration of dissoluted air within permeation water and pressure level imposed within the permeation system. In any case, nominal value for the compressibility of water is much smaller than the compressibility of a permeation system. Although detailed information about pore pressure was not reported, Neuzil et al. [13] indicated that the compressibility of their permeation test system exceeded the nominal value for water by a factor of approximately 100. Similar facts were also reported by Zhang et al. [14] when testing specimens under a pore pressure of 0.1 MPa using syringe pumps and stainless steel lines. Therefore, it is very important to determine experimentally, not theoretically, the values of compressibility of permeation system under identical test conditions. The use of nominal values for the compressibility of water to calculate the value of permeability by using simplified approach may significantly underestimate the permeability. Since a nominal value for the compressibility of water was used to calculate the value of permeability in Brace et al. [8], actual values of permeability of Westerly granite would be at least several orders of magnitude greater than those reported by Brace et al. [8].

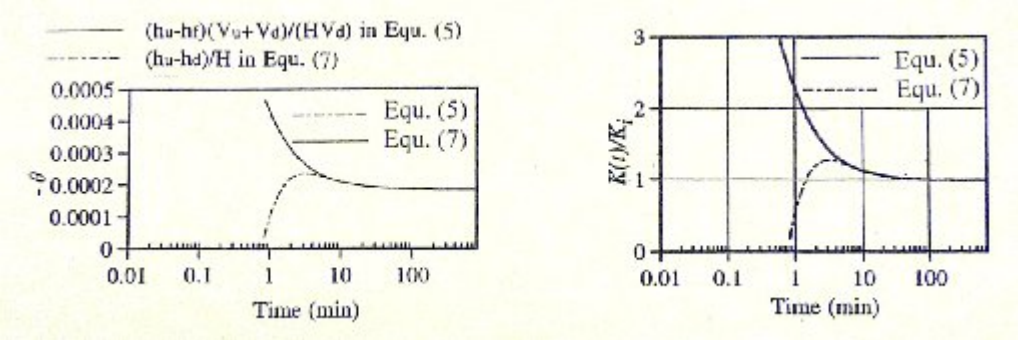
Although a rigorous solution to the transient pulse permeability test has been available since Hsieh et al. derived it in 1981, many researchers still prefer using the method originally proposed by Brace et al.[8] because the latter calculation is much simpler than the rigorous solution. Since the specific storage is not considered in Brace's method, an examination of the effects of specific storage on test results is of fundamental importance. Here we assume a test specimen having the following parameters :

A=1.96 x10^{-3} m^2, L=0.1m, K=1x10^{-11}m/s, S_s=1x10^{-6} 1/m

The compressive storagies of the upstream and downstream permeation sytems are identical, and equal to 4.239x10^{-12} m^2

The pressure decay of a hypothetical transient pulse permeability test can be generated by substitute the above values for related parameters into equation (3). The values of $-\theta$ can be determined from equation (5) or (7), and are plotted versus the log of time, as illustrated in Fig. 3 a). The time dependent value of the permeability, *K(t)*, is plotted versus the log of time in Fig. 3 b), with a ratio to the value of permeability input for generating the hypothetical permeability test, K_i. It is obvious that $-\theta$ is not constant, but time dependent. This time dependency is due to the effects of specific storage. To obtain relatively reliable value for the permeability by means of Brace's method, the use of later part of experimental records is suggestible.

As expressed in equation (6), several parameters are involved in the calculation. The use of different unit system, or misuse of units for any parameters, may induce possible mistakes. Careful examination of the units for individual parameters is of fundamental necessary to ensure the reliability of a calculation, and thus the reliability of the value of permeability.



a) (left) $-\theta$ versus log time curves generated from the hypothetical transient pulse permeability test

b) (right) Time dependent error of permeability

Fig. 3 Time dependent error of using simplified method to determine permeability from a pulse test

Examination of Through-Diffusion Test

Rigorous solution to the through-diffusion test considering concentration decrease in source cell and concentration increase in measurement cell can be obtained by solving the equation (2) together with the initial and boundary conditions illustrated in Fig. 2 b) (lower part) as follows:

$$c(x,t)=\frac{c_1}{\delta+\upsilon+1}- 2c_1\sum_{m=0}^{\infty}\frac{\exp\left(-\frac{D_e\cdot\varphi_m^2}{\alpha\cdot L^2}\cdot t\right)\cdot\left[\delta\cdot\cos\left(\varphi_m\cdot\frac{L-x}{L}\right)-\upsilon\cdot\varphi_m\cdot\sin\left(\varphi_m\cdot\frac{L-x}{L}\right)\right]}{\left[\upsilon\cdot\varphi_m^2-\delta(\delta+\upsilon+1)\right]\cos(\varphi_m)+\left[\delta\cdot\upsilon+\delta+2\upsilon\right]\varphi_m\cdot\sin(\varphi_m)} \quad (8)$$

where $\delta=(\alpha\cdot A\cdot L)/V_u$, $\upsilon=V_d/V_u$ and φ_m are the roots of the following equation:

$$\tan(\varphi)=\frac{\delta\cdot(\upsilon+1)\cdot\varphi}{\upsilon\cdot\varphi^2-\delta^2} \quad (9)$$

Variations in source and measurement cells, i.e., $c(0,t)$ and $c(L,t)$, can be calculated by substituting x = 0 and $x = L$ into equation (8).

Equations (8) and (9) are basically similar to equations (3) and (4), noting that the direction of x is defined from the downstream side towards upstream side in transient pulse permeability test, whereas the direction of x is defined from the source cell side towards measurement cell side in through-diffusion test according to common practice. Due to this similarity, the solution to the transient pulse permeability test can easily be used to interpret the results from through-diffusion tests by simply replacing the hydraulic head, permeability and specific storage with the concentration, effective diffusion coefficient and rock capacity factor, respectively. Inversely, the solution to the through-diffusion test can also be easily used to interpret the transient pulse permeability test by replacing relevant parameters [12].

Conventional through-diffusion test assumes constant concentration in the source cell, and zero concentration in the measurement cell (Fig. 2 b, upper part).

The solution for the conventional type of diffusion test can be obtained as follows [15]:

$$c(x,t) = c_1\left[1 - \frac{x}{L} - \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\cdot\sin\left(n\cdot\pi\cdot\frac{x}{L}\right)\cdot\exp\left(-\frac{n^2\cdot\pi^2\cdot D_e}{\alpha\cdot L^2}\cdot t\right)\right] \tag{10}$$

The total or accumulated quantity $Q(t)$ diffused into the outlet side reservoir, or measurement cell, after time *t* can be calculated as the time integral of the flux through the boundary $x = L$, and can be derived as follows:

$$\begin{aligned} Q(t) &= -D_e\cdot A\int_0^t \frac{\partial(x,\tau)}{\partial x}\Big|_{x=L} d\tau \\ &= A\cdot L\cdot c_1\left\{\frac{D_e}{L^2}\cdot t - \frac{\alpha}{6} - \frac{2\alpha}{\pi^2}\sum_{n=1}^{\infty}\frac{(-1)^n}{n}\exp\left(-\frac{n^2\cdot\pi^2\cdot D_e}{\alpha\cdot L^2}\cdot t\right)\right\} \end{aligned} \tag{11}$$

At long times, the exponential function in equation (11) approaches zero. Consequently, $Q(t)$ at $t\to\infty$ or at the steady state approaches the linear relation

$$Q(t)\Big|_{t\to\infty} = A\cdot L\cdot c_1\left[\frac{D_e}{L^2}\cdot t - \frac{\alpha}{6}\right] \tag{12}$$

with a slope of $(A\cdot c_1\cdot D_e)/L$ and an intercept on the time axis $(\alpha\cdot L^2)/(6D_e)$. By plotting the $Q(t)$ versus *t* curve and obtaining the slope at steady state measurement and the corresponding intercept on the time axis, both the effective diffusion coefficient, D_e, and rock capacity factor, α, can be determined. This method for determining the effective diffusion coefficient and rock capacity factor is known as time-lag method.

To say exactly, equation (11) and (12) are only applicable to the interpretion of through-diffusion tests performed under constant inlet concentration and zero outlet concentration conditions. In practice, however, it is not possible to control the zero concentration in the measurement cell. To detect or analyze the tracer diffused into the measurement cell, the concentration of the tracer in the measurement cell should be allowed to increase to a certain level compared to the sensitivity and precision of the chemical analysis equipment. Otherwise, chemical analysis would be impossible, or the resolution could not be assured.

Quantitative evaluation of the errors associated with using equation (11) together with the time-lag method can be performed by generating a hypothetical through-diffusion test results using the rigorous solution (equation 8), back-calculating the values of effective diffusion coefficient and rock capacity factor with equation (11) and the time-lag method, and comparing the differences between the back-calculated and input values for the two parameters. Table I tabulates the hypothetical test conditions for the theoretical simulation of a through-diffusion test.

Table I Hypothetical test conditions for the theoretical simulation of a through-diffusion test

Specimen	Cross-sectional area, *A* (m^2)	3.85E-3
	Length, *L* (m)	1.00E-2
	Effective diffusion coefficient, D_e (m^2/s)	2.50E-13
	Rock capacity factor, α	3.50E-2
Source cell	Volume, V_u (m^3)	4.00E-6
	Concentration, c (ppm)	1.27E+5
Measurement cell	Volume, V_d (m^3)	4.00E-5
	Concentration, c (ppm)	---

Relative errors in determining effective diffusion coefficient and rock capacity factor by using the time-lag method are tabulated in Table II, in which the relative errors are defined as follows:

$$D_{e-err} = \frac{D_{e-\det ermined}}{D_{e-input}} \cdot 100\% \qquad \alpha_{err} = \frac{\alpha_{\det ermined}}{\alpha_{input}} \cdot 100\% \tag{13}$$

The subscripts determined and input refer, respectively, to the data back-calculated with the time-log method and input for generating hypothetical through-diffusion test using equation (8), respectively.

Table II Relative errors in determining effective diffusion coefficient and rock capacity factor by using the time-lag method

	$1\%c_1$	$3\%c_1$	$5\%c_1$	$9\%c_1$
$D_{e-err}\,(\%)$	96	96	94	88
$\alpha_{err}\,(\%)$	93	90	73	26

If the solution in the measurement cell is not replaced with fresh solution to maintain the zero concentration condition at the outlet end of specimen, and the data are interpreted using the conventional time-lag method, there will be a tendency to underestimate both the effective diffusion coefficient and rock capacity factor. The higher the concentration increase in the measurement cell, the larger will be the error in estimating the two parameters.

CONCLUDING REMARKS

Safety assessment of facilities associated with geological disposal of hazardous waste, including radioactive nuclear waste, is generally performed through mass transport simulations combined with uncertainty and sensitivity analyses. To reduce the uncertainty of a simulation, mathematical models describing the mechanisms of mass transport in a geological formation and boundary conditions describing the geological and hydrogeological conditions for the site should be appropriate. In addition, the values of parameters input for the simulation should be representative of those under in situ conditions.

Although permeation, diffusion and batch experiments have long been used in practice, and are considered to be well-established, they do not necessarily provide accurate values of parameters to be determined without careful examination of calculation methods, resolution of sensors and analytical equipments, and/or test conditions.

Taking the transient pulse permeability test and the through-diffusion test as examples, this paper discussed the major factors that may cause errors in parameter determination. Major conclusions drawn from this study can be summarized as follows:

1) Although it is not a technical problem, negligence or some simple mistakes could be easily made in a calculation due to the use of different unit systems and/or mathematical functions when interpreting transient pulse permeability tests.

2) Neglecting the effects of specific storage may overestimate or under estimate the permeability from a pulse test, depending on the relationships between the storage capacities of the specimen and reservoirs used for transient pulse permeability tests.

3) Compressibility of a permeation system is significantly larger than the nominal values for water due to the mechanical compliance of the equipment. The use of nominal values for the compressibility of water to calculate the value of permeability by using simplified approach may significantly underestimate the permeability.

4) The use of simplified solution together with the conventional time-lag method may underestimate both the effective diffusion coefficient and rock capacity factor. The higher the concentration increase in the measurement cell, the larger will be the error in estimating the two parameters.

5) To obtain reliable values for related parameters, caution should be exercised when interpreting data derived from the transient pulse permeability test and the through-diffusion test.

The findings and conclusions obtained in this study may offer some practical considerations for effective implementations of laboratory permeation and diffusion tests, proper interpretation of test results, examination and/or proper citation of the data reported in existing articles for a scientific simulation.

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